

N,N,N',N',N'',N''-Hexakis(methoxymethyl)-1,3,5-triazine-2,4,6-triamine
3089-11-0 | DTXSID9027520

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 5.11e-07 mmHg

Global applicability domain: Outside

Local applicability domain index: 1.82e-01

Confidence level: 3.81e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Indanofan</div> <div>Measured: 2.30e-07</div> <div>Predicted: 3.60e-08</div>	<div>Image not found</div> <div>Coumaphos</div> <div>Measured: 9.70e-08</div> <div>Predicted: 2.52e-07</div>	<div>Image not found</div> <div>Flubenzimine</div> <div>Measured: 8.00e-05</div> <div>Predicted: 2.90e-06</div>
<div>Image not found</div> <div>2-Chlorobenzoic acid</div> <div>Measured: 1.10e-08</div> <div>Predicted: 3.25e-03</div>	<div>Image not found</div> <div>Oxamyl</div> <div>Measured: 2.90e-06</div> <div>Predicted: 1.05e-04</div>	